# A turbulent mixing
# Reynolds Stress Model
# fitted to match
# Linear Interaction Analysis predictions.

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# Scope of the study

### General purpose

Search for a Reynolds Stress Model (RSM) able to predict the evolution of turbulent mixing zones in shock tube experiments with different gases.

$\hookrightarrow$ need for correct evaluation of the production due to
**shock wave / turbulent mixture interaction**.

### Model under consideration

One-point RSM with additional equations for

- variance of the specific volume (inverse of density)

- density-velocity correlation;

$\hookrightarrow$ modified **GSG model** with variables $\widetilde{R_{ij}}, \overline{v_i''}, \widetilde{\tau''^2}, \tilde{\varepsilon}$
$$(\textit{i.e. } \widetilde{v_i''v_j''}, \widetilde{v_i''\tau''}, \widetilde{\tau''\tau''}, \tilde{\varepsilon})$$

(O. Grégoire, D. Souffland and S. Gauthier, *J. of Turbulence* 6(29), 2005).

# Scope of the study

## Limited purpose

Deriving a Reynolds Stress Model (RSM) able to predict the turbulent quantities downstream from a shock front crossing an **homogeneous turbulent mixture** (statistically stationnary and 0D problem).
(Limitation to upstream turbulent fields representative of turbulent mixing layers.)

## Assumptions and simplifications

- **Linearity** of upstream perturbations *i.e.* "weak" turbulence

- Interactions are quick enough so that turbulent **diffusion and dissipation are negligible** during the shock-turbulence interaction.

- **Pseudopressure** formulation based numerical implementation

## Ingredients to be used

**LIA** : Linear Interaction Analysis (interaction with shock waves)
**PDF** : Probability Density Function models (to derive consistant RSM)

# Summary

1. Linear Interaction Analysis

2. Transfer matrices

3. Probability Density Function based RSM

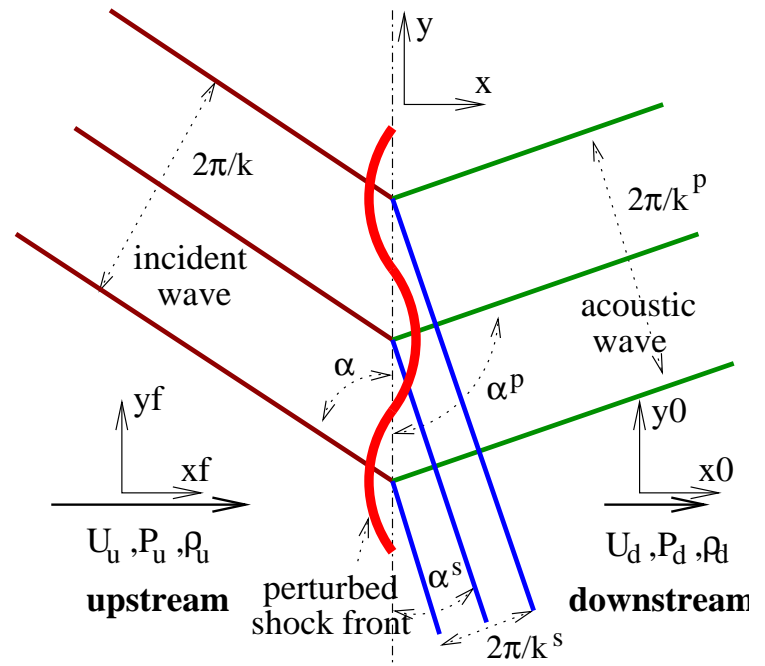4. Model improvement

# Part I :
# Linear Interaction Analysis

# Linear Interaction Analyis

## Kovasznay decomposition

thanks to linearity, perturbation fields are decomposed into entropy, vorticity and acoustic waves upstream of and downstream from the shock front.

## Picture of the interaction  of a single non-acoustic wave with a shock front.

all non-acoustic waves (the transmitted one and the created ones) are advected with material speed and remain completely correlated.
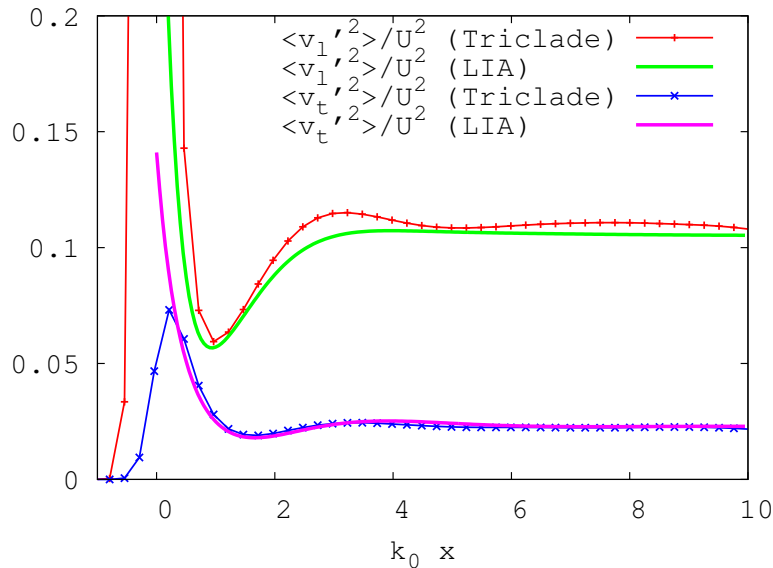
## Transfer functions

$Z_{it}(\alpha)$ relates the amplitude of the downstream wave family of kind $t$ (transmitted) to the upstream perturbation of kind $i$ (incident).
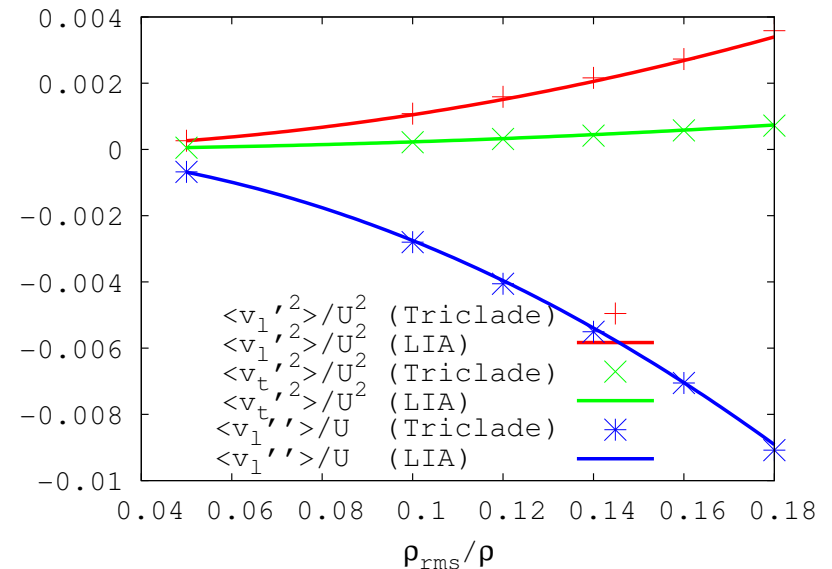
# Shock wave / mixture interaction

Interaction of a Mach 2 shock wave with a mixture of gases at rest

Comparison: symbols- numerical simulation (TRICLADE), solid lines- LIA.



Downstream profile



Far-field values

- good agreement between LIA and numerical simulation.

- 2 regions downstream: a near-field and a far-field.

Goal: the GSG model should reproduce the far field values.

# Part II :
# Transfer matrices

# Special upstream turbulent field

Restriction to a particular class of upstream fields

obtained as a sum of plane waves (entropy, index $d$, and vorticities, indices $v, w$) with the main specificities encountered in turbulent mixing zones :

$$\left( \frac{\hat{\rho}}{\bar{\rho}}, \frac{\hat{v}_x}{V_{ref}}, \frac{\hat{v}_r}{V_{ref}}, \frac{\hat{v}_\theta}{V_{ref}}, \frac{\hat{p}}{\bar{P}} \right) (k, \alpha, \phi) =$$

$$(\hat{a}_d(k, \alpha, \phi), \hat{a}_v(k, \alpha, \phi) \sin\alpha, -\hat{a}_v(k, \alpha, \phi) \cos\alpha, \hat{a}_w(k, \alpha, \phi), 0)$$

with

$$\forall i, j \in \{d, v, w\}, \qquad \langle \hat{a}_i \hat{a}_j^* \rangle (k, \alpha, \phi) = \langle \hat{a}_i \hat{a}_j^* \rangle_\alpha(\alpha) \times \langle \hat{a}_i \hat{a}_j^* \rangle_k(k)$$

- hypothesis of axisymmetry;

- hypothesis of separability of dependence on wavenumber $k$ and incidence angle $\alpha$;

- no acoustic waves (emitted out of thin mixing layers);

- turbulent mass flux due to correlation between entropy and vorticity modes;

- isotropy if functions of $\alpha$ are constant and $\langle |\hat{a}_v|^2 \rangle = \langle |\hat{a}_w|^2 \rangle$;

Thanks to LIA, the corresponding downstream field is completely determined (for each upstream Fourier component).

# Transfer matrices

## Relation to GSG model variables

The following nondimensional vector of variables used by the GSG model is considered

$$X = \left( \frac{\widetilde{R_{xx}}}{\tilde{c}^2}, \frac{\overline{v_x''}}{\tilde{c}}, \frac{\widetilde{\tau''^2}}{\tilde{\tau}^2}, \frac{\widetilde{R_{tt}}}{\tilde{c}^2} \right) \qquad \text{with } \tilde{c} \text{ sound celerity}$$

With given shape of functions $\langle \hat{a}_i \hat{a}_j^* \rangle_\alpha (\alpha)$, upstream values of $X$ are given.
These functions are assumed constant (independance on the incidence angle $\rightarrow$ true in the isotropic limit).

## Transfer matrix from linear theories

Then, unique identification of a **transfer matrix** between upstream and downstream turbulent mixture can be obtained from linear results (LIA)

$$X_{downstream} = S_{LIA}.X_{upstream}$$

The transfer matrix *only depends on the density ratio* accross the rarefaction fan or shock front *and the adiabatic index* $\gamma$ of the gases.

$$\text{example}: S_{13} = \int_0^{\pi/2} \sin^2 \alpha^s |Z_{sv}|^2 \sin \alpha \mathrm{d}\alpha:$$

longitudinal Reynolds stress production by upstream density variance.

# Solution for the GSG model

Production by the mean flow in the original GSG model

$$\bar{\rho}\frac{\partial \widetilde{R_{xx}}}{\partial t} + \bar{\rho}\tilde{v}_x\frac{\partial \widetilde{R_{xx}}}{\partial x} = -2(1-\tfrac{2}{3}\gamma')\bar{\rho}\widetilde{R_{xx}}\frac{\partial \tilde{v}_x}{\partial x} - 2(1-\tfrac{2}{3}\gamma^H)\overline{v''_x}\frac{\partial \bar{P}}{\partial x}$$

$$\bar{\rho}\frac{\partial \widetilde{R_{tt}}}{\partial t} + \bar{\rho}\tilde{v}_x\frac{\partial \widetilde{R_{tt}}}{\partial x} = -\tfrac{2}{3}\gamma'\bar{\rho}\widetilde{R_{xx}}\frac{\partial \tilde{v}_x}{\partial x} - \tfrac{2}{3}\gamma^H\overline{v''_x}\frac{\partial \bar{P}}{\partial x}$$

$$\frac{\partial \overline{\rho'^2}}{\partial t} + \tilde{v}_x\frac{\partial \overline{\rho'^2}}{\partial x} = -2\overline{\rho'^2}\frac{\partial \tilde{v}_x}{\partial x} + 2\bar{\rho}\overline{v''_x}\frac{\partial \bar{\rho}}{\partial x}$$

$$\frac{\partial \overline{v''_x}}{\partial t} + \tilde{v}_x\frac{\partial \overline{v''_x}}{\partial x} = -(1-\gamma^u)\overline{v''_x}\frac{\partial \tilde{v}_x}{\partial x} + (1-\gamma^u)\frac{\widetilde{R_{xx}}}{\bar{\rho}}\frac{\partial \bar{\rho}}{\partial x} - (1-\gamma^u)\frac{1}{\bar{\rho}}\frac{\overline{\rho'^2}}{\bar{\rho}^2}\frac{\partial \bar{P}}{\partial x}$$

Looking for a (continuous) stationnary solution yields

$$\mathfrak{m}\frac{dX}{d\mathfrak{m}} - M_{GSG}.X = 0$$

where $\mathfrak{m}$ is the local compression ratio and $M_{GSG}$ is a *constant matrix* known from the model coefficients.

$$M_{GSG} = \begin{pmatrix} 2(2-\tfrac{2}{3}\gamma') & -2(1-\tfrac{2}{3}\gamma^H) & 0 & 0 \\ 1-\gamma^u & 2-\gamma^u & -(1-\gamma^u) & 0 \\ 0 & 2 & 0 & 0 \\ \tfrac{2}{3}\gamma' & -\tfrac{2}{3}\gamma^H & 0 & 2 \end{pmatrix}$$

# Pseudopressure

## Pseudopressure based numerical implementation

- Pressure $p$ + pseudopressure $q$ substituted to $p$ in mean momentum and energy equations but *not* in the equation of state;

- Typical form: $q = -c_1 \rho c L (\vec{\nabla}.\vec{v}) + c_2 \rho L^2 (\vec{\nabla}.\vec{v})^2$ if $\vec{\nabla}.\vec{v} < 0$, $q = 0$ otherwise;

- Effect: "shock fronts" are described as **continuous** variations with non-zero finite thickness.

In a stationnary shock front, $\bar{q}/\bar{p}$ is a known function of $\mathfrak{m}$ (local compression ratio) and $\mathcal{M}_0$ (shock Mach number) **whatever** its definition (values of $c_1$ or $c_2$ for instance).

## Modified GSG with pseudopressure based numerical implementation

The relation for continuous stationnary solution

$$\mathfrak{m}\frac{dX}{d\mathfrak{m}} - M_{GSG*}.X = 0$$

holds for modified GSG with $M_{GSG*}$ depending on $\bar{q}/\bar{p}$ (*i.e* depending on $\mathfrak{m}$).
Thanks to numerical pseudopressure, in the frame moving with the mean shock celerity, the shock / (homogenous weak) turbulence mixture interaction is a statistically continuous stationnary problem so that *turbulence evolution across a shock front is described by the previous relation*.

# RSM transfer matrix

## From matrix $M_{GSG^*}$ to RSM transfer matrix $S_{GSG^*}$

So with $m$ the total compression ratio, for every upstream turbulent field, equation

$$\mathfrak{m}\frac{dX}{d\mathfrak{m}} - M_{GSG^*}.X = 0$$

yields the downstream value of $X$ after integration on $\mathfrak{m}$ from 1 (upstream) to $m$ (downstream).

Using linearity of the relation leads to the **transfer matrix** $S_{GSG^*}$

$$X_{downstream} = S_{GSG^*}.X_{upstream}$$

$\hookrightarrow$ validity whatever the pseudopressure.
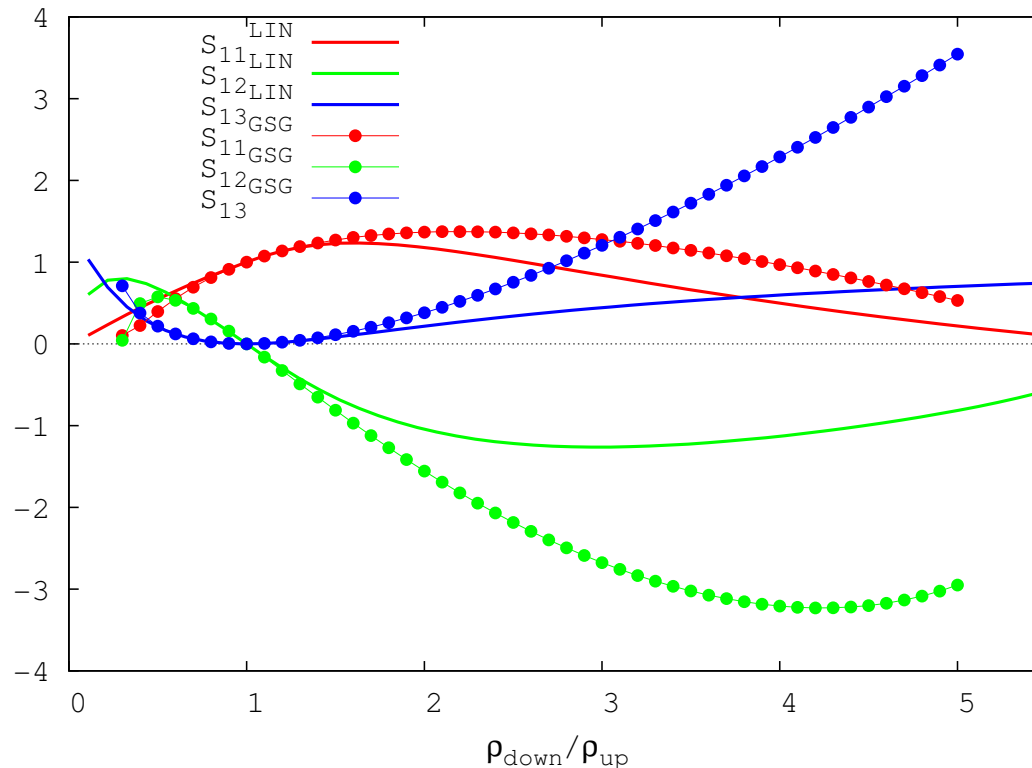
$\hookrightarrow$ (quasi-)independence on the adiabatic index (contrary to LIA).

Recall (normalization by local values):

$$X = \left( \frac{\widetilde{R_{xx}}}{\tilde{c}^2}, \frac{\widetilde{v_x''}}{\tilde{c}}, \frac{\widetilde{\tau''^2}}{\tilde{\tau}^2}, \frac{\widetilde{R_{tt}}}{\tilde{c}^2} \right) \qquad \text{with } \tilde{c} \text{ sound celerity}$$

# Transfer matrix comparison

Contribution to longitudinal Reynolds stress ($\gamma = 7/5$)

with respect to the compression ratio ($m = 6$ for infinitely strong shock)



$\hookrightarrow$ large discrepancies with the original GSG model in the limit of strong shocks ($m \to 6$) or strong rarefactions ($m \to 0$).

In particular, the effect of upstream density contrast $S_{13}$ is largely overpredicted by the model even at moderate shock strength (important in shock tube applications).

# Improvement purpose

## Target

For modified GSG, the evolution of a (weakly) turbulent field across a shock front is completely described by $S_{GSG^*}$.

The reference evolution, considered as the "true" one, is given by $S_{LIA}$.

$\hookrightarrow$ correct the GSG model in shock front in such a way that

$$S_{GSG^*} \textbf{ remain "close" to } S_{LIA}$$

*whatever* $\mathcal{M}$ (shock Mach number) or $\gamma$ (adiabatic index).

Corrections should maintain consistency between the different equations and **preserve realizability**.

$\hookrightarrow$ derive RSM from a PDF model.

# Part III :

# Probability Density Function based RSM

# Probability Density Function based RSM

Stochastic PDE for Favre fluctuations

$$\frac{du_i''}{dt} = -u_k''\left[\partial_k \tilde{U}_i\,(1-8\alpha_1) + 2\alpha_1\partial_i\tilde{U}_k\right]$$
$$-\tfrac{1}{2}\left(4\alpha_1 div\tilde{U} + \Omega_R + C_1\omega\right)u_i''$$
$$-\partial_i\bar{P}\tau''\,(1-A_1) + \sqrt{(C_0\omega+\Omega_W)\tilde{k}}\dot{W}_i$$

$$\frac{d}{dt}\left(\frac{\tau''}{\tilde{\tau}}\right) = -u_k''\frac{\partial_k\tilde{S}}{c_p} - \frac{C_\rho}{2}\omega\frac{\tau''}{\tilde{\tau}} - \sqrt{C_{\rho 0}\,\omega\,\frac{\widetilde{\tau''^2}}{\tilde{\tau}^2}}\dot{W}_\rho$$

$$\frac{dx_i}{dt} = \tilde{U}_i + u_i''$$

with $\omega = \tilde{\varepsilon}/\tilde{k}$ the turbulent frequency, $b_{ij} = \tilde{R}_{ij}/(2\tilde{k}) - \delta_{ij}/3$ and

$$\Omega_R = \max\left(0\,,\; 12\alpha_1 b_{kl}\partial_l U_k + A_1\frac{\partial_k\bar{P}}{\bar{\rho}}\frac{\overline{u_k''}}{\tilde{k}} + (1-C_1)\,\omega\right)$$

$$\Omega_W = \tfrac{2}{3}\left(\Omega_R - 12\alpha_1 b_{kl}\partial_l U_k - A_1\frac{\partial_k\bar{P}}{\bar{\rho}}\frac{\overline{u_k''}}{\tilde{k}}\right)$$

$$C_0 = \frac{2}{3}\,(C_1-1)\quad C_\rho = 2C_{u_2} - C_1\quad C_{\rho 0} = C_\rho - C_{\rho 2}$$

$W_i$ and $W_\rho$ are independent Brownian processes.

$\hookrightarrow$ gives equations for $\widetilde{v_i''v_j''}, \widetilde{v_i''\tau''}, \widetilde{\tau''\tau''}$ (up to triple correlations that are closed with classical turbulent diffusion hypotheses), cf S.B. Pope.

# Properties of PDF based RSM

## Properties of the resulting RSM

- ensures compatibility of equations for $\widetilde{v_i'' v_j''}, \widetilde{v_i'' \tau''}, \widetilde{\tau'' \tau''}$;

- ensures realizability (up to the diffusion terms) :

  positivity of $\widetilde{v_i''^2}, \widetilde{\tau''^2}$ and

  Schwarz inequality $\overline{v_i''}^2 \leq \bar{\rho}^2 \widetilde{\tau''^2} \tilde{R}_{ii}$  (i.e. $\widetilde{v_i'' \tau''}^2 \leq \widetilde{v_i''^2} \widetilde{\tau''^2}$)

- the production by the mean flow is defined by only 2 parameters : $\alpha_1$ and $A_1$.

These good properties are preserved even if the parameters $\alpha_1$ and $A_1$ are modified.
$\hookrightarrow$ natural way to induce a special evolution of the turbulence inside shock fronts.

# Part IV :
# Model improvement

# Frame of improvement

## Recall : goal

Correction in order that $S_{GSG*}$ remain "close" to $S_{LIA}$
_whatever_ $\mathcal{M}$ (shock Mach number) or $\gamma$ (adiabatic index).

## Frame

Corrections introduced in the stochastic PDE to derive a consistant and realizable RSM. The ratio $\bar{q}/\bar{p}$ becomes significant only inside shock fronts (it distinguishes compression ramps from shock waves).
Two coefficients related to the production by mean flow can be modified inside "shocks" :

$$A_1 \rightarrow A_1(\bar{q}/\bar{p}) \qquad \alpha_1 \rightarrow \alpha_1(\bar{q}/\bar{p})$$

$\hookrightarrow$ not sufficient, an important improvement comes from taking the pseudopressure into account in the derivation of the model for the fluctuating velocity divergence.

# Divergence of fluctuating velocity

## Without pseudopressure

In the original GSG model, correlations involving $\mathrm{div}\vec{v}'$ are treated as dissipation terms so they vanish in the limit considered here.

A low Mach number model ($\approx$ hyp. $p'/\bar{p} = 0$) shows that in the present case

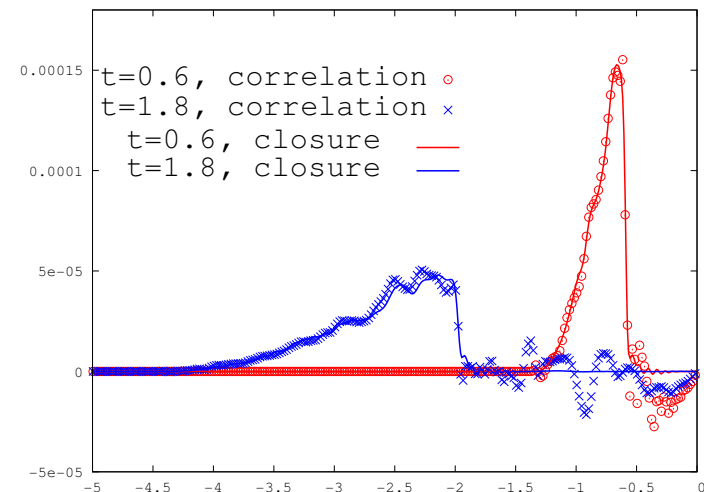$$\mathrm{div}\vec{v}' = -\vec{v}''.\frac{\vec{\nabla}\bar{p}}{\gamma\bar{p}} + \mathcal{F}$$

- the second term is diffusive ;
- the first part, not taken into account in the original GSG model, leads to the main improvements of the modified one.

$\hookrightarrow$ this amounts to treat the density fluctuation as an active scalar instead of a passive one in the original derivation in the GSG model.

Interaction between rarefaction fan and mixture at rest (two times). Comparison of correlation $\overline{v_x''\mathrm{div}\vec{v}''}$ :
-simulation results (symbols)
-closed with low Mach number model (lines).

# Divergence of fluctuating velocity

With a pseudopressure taken into account

If $\quad q = -\rho^n (\lambda/\rho^n)\vec{\nabla}.\vec{v} \quad$ with $\quad \lambda/\rho^n = constant \quad$ then $\quad q' = \bar{q}\left( n\frac{\rho'}{\bar{\rho}} + \frac{\vec{\nabla}.\vec{v}'}{\vec{\nabla}.\vec{v}} \right)$

(corresponds to bulk viscosity with prescribed $\lambda$ dependance on temperature and given thermodynamic path).

Assuming $p'/\bar{p} = 0$ leads to

$$\vec{\nabla}.\vec{v}' = -\frac{\vec{\nabla}\bar{p}}{\gamma\bar{p}}.\vec{v}'' + \frac{\kappa}{1+\kappa}\left( \frac{n}{2}\vec{\nabla}.\vec{v}\frac{\tau''}{\tilde{\tau}} + \frac{\vec{\nabla}\bar{p}}{\gamma\bar{p}}\vec{v}'' \right) \quad \text{with} \quad \kappa = 2\frac{\gamma-1}{\gamma}\frac{\bar{q}}{\bar{p}}$$

The only corrected stochastic PDE is

$$\frac{d}{dt}\left( \frac{\tau''}{\tilde{\tau}} \right) = -\frac{\vec{\nabla}\tilde{S}}{c_p}.\vec{v}'' + \frac{\kappa}{1+\kappa}\left( \frac{n}{2}\vec{\nabla}.\vec{v}\frac{\tau''}{\tilde{\tau}} + \frac{\vec{\nabla}\bar{p}}{\gamma\bar{p}}.\vec{v}'' \right) - \frac{C_\rho}{2}\omega\frac{\tau''}{\tilde{\tau}} - \sqrt{C_{\rho_0}\omega\frac{\widetilde{\tau''^2}}{\tilde{\tau}^2}}\dot{W}_\rho$$

# Coefficient optimization

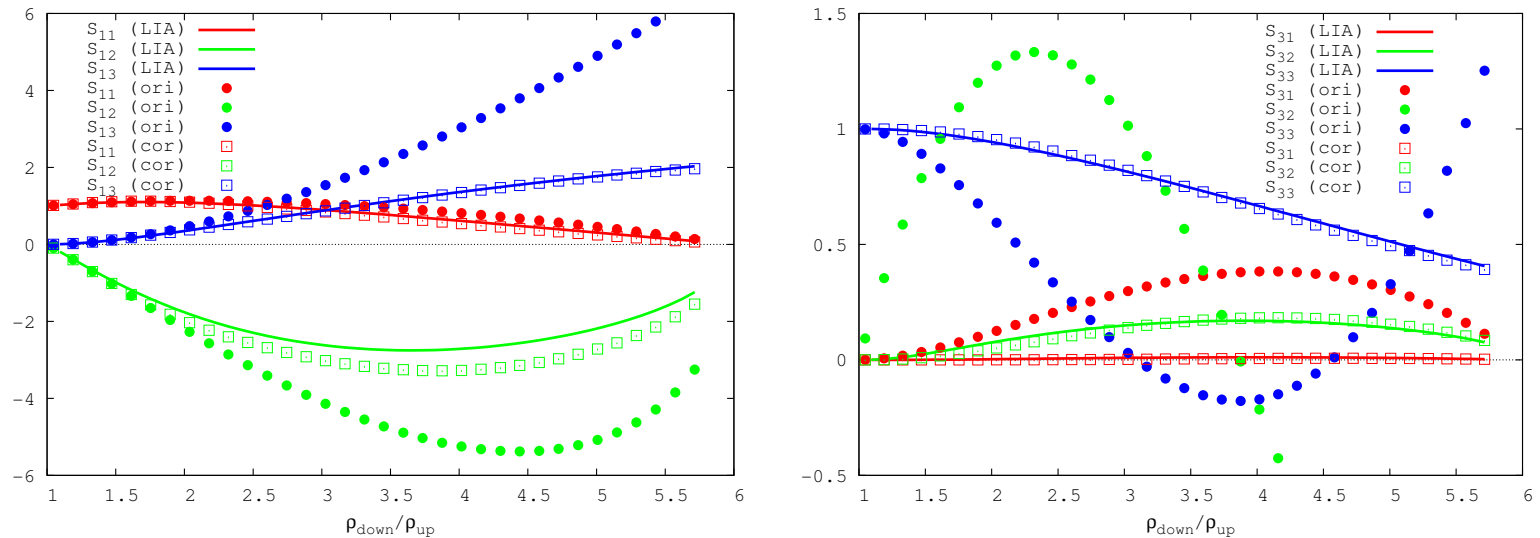With fluctuating pseudopressure taken into account ($n = 0.6$), assume

$$A_1 = \frac{3}{10} + \frac{c_A}{\gamma}\chi \quad \alpha_1 = \frac{1}{10} + \frac{c_\alpha}{\gamma}\chi \quad \text{with} \quad \chi = \frac{\bar{q}/\bar{p}}{0.15 + \bar{q}/\bar{p}}$$

Minimization of a norm $||S_{SGS} - S_{LIA}||$ gives the range of optimal coefficients $c_A$ and $c_\alpha$ for every shock Mach numbers. We choose $c_A = 0.46$ and $c_\alpha = 0.2$.

# Transfer matrix comparison

Contributions to kinetic energy (left) and density variance (right)
with respect to the compression ratio ($m = 6$ for infinitely strong shocks $\gamma = 7/5$)



lines : LIA, filled circles: original GSG, squares: corrected GSG

$\hookrightarrow$ large improvement especially concerning density variance production and turbulent mass flux (not shown).

# Conclusions (1/2)

## Summary of the method

Obtain, from both LIA and RSM, matrices connecting values of quantities involved in the one-point turbulence model upstream of and downstream from a shock wave (also possible with rarefaction fans).
Transfer matrix computation requires:

- for RSM : pseudopressure numerical implementation

- for LIA : "weak" turbulence and restriction of upstream fields

## Prescriptions for turbulence modelling

Compatibility of RSM with LIA requires that *both transfer matrices remain close* for all shock Mach number and adiabatic indices.

# Conclusions (2/2)

## Modelization improvement

**Optimization frame** :

use of RSM deduced from *PDF models* with small number of parameters

$\hookrightarrow$ ensures realizability

**Numerical pseudopressure** $\bar{q}$ :

distinguishes compression ramps from shock waves.

It can be used in two ways

- make the (relevant) parameters dependent on the ratio $\bar{q}/\bar{p}$;
- take the effect of $\bar{q}$ into account in the fluctuating divergence velocity model.

Fits using both ways allow to write shock corrections giving RSM results reasonnably close to LIA ones for all shock Mach numbers and polytropic indices.

## Future work

Such an optimization is possible for the dissipation equation but non-equilibrium effects due to spectrum reorganization *after* shock interaction must be modelled.